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Threshold properties of attractive and repulsive $1/r^2$ potentials

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We study the near-threshold ($E \rightarrow 0$) behavior of quantum systems described by an attractive or repulsive $1/r^2$ potential in conjunction with a shorter-ranged $1/r^m$ ($m>2$) term in the potential tail. For an attractive $1/r^2$ potential supporting an infinite dipole series of bound states, we derive an explicit expression for the threshold value of the pre-exponential factor determining the absolute positions of the bound-state energies. For potentials consisting entirely of the attractive $1/r^2$ term and a repulsive $1/r^m$ term, the exact expression for this prefactor is given analytically. For a potential barrier formed by a repulsive $1/r^2$ term (e.g., the centrifugal potential) and an attractive $1/r^m$ term, we derive the leading near-threshold behavior of the transmission probability through the barrier analytically. The conventional treatment based on the WKB formula for the tunneling probability and the Langer modification of the potential yields the right energy dependence, but the absolute values of the near-threshold transmission probabilities are overestimated by a factor which depends on the strength of the $1/r^2$ term (i.e., on the angular momentum quantum number l) and on the power m of the shorter ranged $1/r^m$ term. We derive a lower bound for this factor. It approaches unity for large l, but it can become arbitrarily large for fixed l and large values of m. For the realistic example $l=1$ and $m=6$, the conventional WKB treatment overestimates the exact near-threshold transmission probabilities by at least 38%.

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I. INTRODUCTION

Encouraged by the interest in cold atoms and their interactions, there has recently been strong activity in the study of atomic and molecular systems near the threshold which separates the bound-state regime from the continuum [1]. The Schrödinger equation for a particle of mass $\mathcal{M}$ in a potential $V(r)$ is

$$\psi''(r)+\frac{2\mathcal{M}}{\hbar^2}[E-V(r)]\psi(r)=0, \quad r>0, \tag{1}$$

and the behavior of its solutions near threshold depends crucially on the asymptotic (large-r) behavior of the potential.

For long ranged potentials falling off slower than $1/r^2$ (e.g., the Coulomb potential), the threshold $E=0$ represents the semiclassical limit [2], and there are infinitely many bound states if the potential tail is attractive. The behavior of the quasicontinuum of bound states just below threshold and the real continuum above threshold is well understood, at least for the case of one Coulombic coordinate, on the basis of quantum defect theory.

For potentials tails falling off faster than $1/r^2$, the threshold $E=0$ represents the anticlassical limit of the Schrödinger equation, and the potential supports at most a finite number of bound states. Near-threshold properties of bound and continuum states for deep potentials with attractive tails falling off faster than $1/r^2$ have been the subject of several recent publications [3–11].

This paper deals with potentials asymptotically proportional to $1/r^2$ which represent the borderline separating the long-range tails from shorter-range tails. For a potential proportional to $1/r^2$, the energy dependence scales out of the Schrödinger equation (1); the semiclassical limit is reached neither for $E \rightarrow 0$ nor for $|E| \rightarrow \infty$, but for large absolute values of the potential strength [2]. Repulsive $1/r^2$ potentials appear commonly as centrifugal potential in the radial Schrödinger equation. An attractive $1/r^2$ potential can occur through the interaction of a charged particle with a permanent electric dipole, as in the scattering of electrons by polar molecules [12] or by excited hydrogen atoms [13–15]. If such an attractive $1/r^2$ potential is sufficiently strong, it supports an infinite ''dipole series'' of bound states [13–17]. Moderately strong attractive $1/r^2$ potentials have been seen as a probable mechanism for the generation of ''quantum halo states'' [18]. If the strength of the (attractive) $1/r^2$ term is too weak, then the potential supports at most a finite number of bound states (see, e.g., Ref [19]).

We study potentials behaving for large r as

$$V(r)=\frac{\hbar^2}{2\mathcal{M}}\left[\frac{\gamma}{r^2}\pm\frac{\beta^{m-2}}{r^m}\right], \quad m>2. \tag{2}$$

The dimensionless strength parameter γ of the $1/r^2$ term can be positive or negative, and for the centrifugal potential in the radial part of the three-dimensional Schrödinger equation with angular momentum quantum number l we have $\gamma=l(l+1)$. The strength of the $1/r^m$ term is expressed in terms of the (non-negative) parameter β, which has the physical dimension of a length.

For $m=4$ the Schrödinger equation with potential (2) posesses analytical solutions based on Mathieu functions [20–22]. More general potentials like Eq.(2) have been studied extensively over the years [23–28], mainly with the aim of understanding scattering properties. In the present paper we focus on two particular features of $1/r^2$ potentials. In Sec. II we study potentials with an attractive $1/r^2$ term strong enough to support an infinite dipole series of bound states, and we calculate the threshold value of the factor determining the absolute values of the energies in the series. In Sec.

III we study potential barriers consisting of a repulsive $1/r^2$ term and an attractive $1/r^m$ term, and we derive the exact expression for the near-threshold behavior of the transmission probability through the barrier. This enables us to give a founded judgement on the accuracy of the conventional procedure for deriving transmission probabilities which is based on the WKB formula and the Langer modification of the potential.

II. DIPOLE SERIES OF BOUND STATES

When the $1/r^2$ term in the potential tail [Eq. (2)] is attractive, we have $g \stackrel{\text{def}}{=} -\gamma > 0$. If the strength parameter g is sufficiently large, *viz.* $g > 1/4$, then the potential supports an infinite "dipole series" of bound states whose energies approach an exponential behavior near threshold [13–17]:

$$E_n \stackrel{n\to\infty}{=} -F \exp\left(-\frac{2\pi n}{\sqrt{g-1/4}}\right). \tag{3}$$

The limiting value of the ratio of successive energies in a dipole series is fixed by the strength of the $1/r^2$ term in the potential tail, and is simply $\lim_{n\to\infty} E_n/E_{n+1} = \exp(2\pi/\sqrt{g-1/4})$. However, the constant of proportionality F in Eq. (3) depends very sensitively on the potential at shorter distances, where it necessarily deviates from the $1/r^2$ behavior.

We first look at the case where the shorter ranged term proportional to $1/r^m$ is attractive. At threshold, $E=0$, the Schrödinger equation (1) with potential (2) is

$$\left[\frac{d^2}{dr^2} + \frac{g}{r^2} + \frac{\beta^{m-2}}{r^m}\right] M(r) = 0. \tag{4}$$

We introduce the abbreviations

$$\tau \stackrel{\text{def}}{=} \sqrt{g - \frac{1}{4}}, \quad \xi \stackrel{\text{def}}{=} \frac{2\tau}{m-2} = \frac{2}{m-2}\sqrt{g-\frac{1}{4}}. \tag{5}$$

Two linearly independent analytical solutions of Eq. (4) are

$$M_{1;2}(r) = \sqrt{r} J_{\pm i\xi}(\rho), \quad \rho \stackrel{\text{def}}{=} \frac{2}{m-2}\left(\frac{\beta}{r}\right)^{(m-2)/2}. \tag{6}$$

Here $J_{\pm i\xi}$ stands for the ordinary Bessel function [29] of order $\pm i\xi$. The asymptotic $(r\to\infty)$ behavior of solutions (6) is

$$M_{1;2}(r) \sim \frac{(m-2)^{\mp i\xi}}{\Gamma(1\pm i\xi)} \sqrt{r} \left(\frac{\beta}{r}\right)^{\pm i\tau} \left(1 - \frac{(\beta/r)^{m-2}}{(m-2)^2(1\pm i\xi)}\right). \tag{7}$$

For sufficiently large r, the shorter-ranged term in the potential tail can be neglected, so the Schrödinger equation for finite negative energy, $E = -\hbar^2\kappa^2/(2\mathcal{M})$, is

$$\left[\frac{d^2}{dr^2} + \frac{g}{r^2} - \kappa^2\right] R = 0. \tag{8}$$

The solutions of Eq. (8) are functions of κr only, and the physically relevant solution is

$$R(\kappa r) = i \exp\left(-\frac{\pi}{2}\tau\right) \sqrt{\kappa r} H^{(1)}_{i\tau}(i\kappa r), \tag{9}$$

which behaves asymptocially $(\kappa r\to\infty)$ as

$$R(\kappa r) \sim \sqrt{\frac{2}{\pi}} \exp(-\kappa r). \tag{10}$$

The function $H^{(1)}_{i\tau}$ in (10) is the Hankel function of order $i\tau$ as defined in Ref. [29],

$$H^{(1)}_{i\tau}(z) = \frac{\exp(\pi\tau) J_{i\tau}(z) - J_{-i\tau}(z)}{\sinh(\pi\tau)}. \tag{11}$$

For sufficiently small values of κ, we may use the small argument expansion of the Bessel functions in Eq. (11) to obtain

$$R(\kappa r) \stackrel{\kappa r\to 0}{\sim} \sqrt{\frac{\kappa r}{\pi\tau \sinh(\pi\tau)}} \left[e^{-i\theta}\left(\frac{\kappa r}{2}\right)^{i\tau} + e^{+i\theta}\left(\frac{\kappa r}{2}\right)^{-i\tau}\right] \times [1 + O((\kappa r)^2)], \tag{12}$$

where $\theta \stackrel{\text{def}}{=} \arg \Gamma(i\tau)$. The r dependence of the leading terms in Eq. (12) is the same as the large-r behavior [Eq. (7)] of the zero-energy wave functions [Eqs. (6)] in the full potential tail [Eq. (2)], so we can determine the near-threshold (real) solution of the Schrödinger equation to order below κ^2 by taking the appropriate superposition of the solutions (6),

$$R(\kappa r) = L M_1(r) + L^* M_2(r) \stackrel{\text{def}}{=} M_\kappa(r). \tag{13}$$

The coefficient L is determined by the condition that the leading asymptotic $(r\to\infty)$ terms derived for Eq. (13) from Eq. (7) agree with the corresponding leading terms in Eq. (12):

$$L = \sqrt{\frac{\kappa}{\pi\tau\sinh(\pi\tau)}} e^{i\theta} \Gamma(1+i\xi)(m-2)^{i\xi} \left(\frac{\kappa\beta}{2}\right)^{-i\tau}. \tag{14}$$

Solutions (6) of the Schrödinger equation (4) at energy zero are accurate as long as the energy term κ^2 is negligible in comparison with the smaller of the two potential terms, which is g/r^2 when the shorter-ranged term is dominant. This implies

$$r \ll \frac{\sqrt{g}}{\kappa}. \tag{15}$$

The Schrödinger equation with the full potential tail can be approximated by its asymptotic form [Eq. (8)], when r is so large that the shorter ranged term β^{m-2}/r^m is negligible compared with the longer-ranged term g/r^2, implying

$$r \gg \frac{\beta}{g^{1/(m-2)}}. \tag{16}$$

We can match the superposition [Eq. (13)] of zero-energy solutions to solutions (9),(12) of Eq. (8) if there is a region of r values, where conditions (16) and (15) are satisfied simultaneously. This is the case when the right-hand side of Eq. (15) is much larger than the right-hand side of Eq. (16), i.e., when

$$\kappa\beta \ll g^{(1/2)+[1/(m-2)]}. \tag{17}$$

In other words, matching is justified in the limit $\kappa \to 0$, which is sufficient to determine the leading near-threshold behavior of the energy eigenvalues. An estimate for the numerical accuracy of the near-threshold formulas derived below cannot, however, be given on the basis of the leading terms alone. For this we would require a knowledge of the next-to-leading terms, for which we would have to include corrections of order E in the wave functions.

As r decreases, the argument ρ in solutions (6) becomes large, and we approximate the near-threshold wave function (13) via the large argument expansion of the Bessel functions [29], $J_{\pm i\xi}(\rho) \sim \sqrt{2/(\pi\rho)}\cos[\rho \mp i(\pi/2)\xi - \frac{1}{4}\pi]$,

$$M_\kappa(r) \overset{r\to 0}{\propto} r^{m/4}\cos\left(\rho - \frac{\pi}{4} + \delta\right), \tag{18}$$

where δ is an angle defined by

$$\tan\delta = \tanh\left(\frac{\pi}{2}\xi\right)\tan\left(\theta + \chi + \frac{\pi}{2} - \tau\ln q\right),$$

$$q = \frac{\kappa\beta}{2(m-2)^{2/(m-2)}}; \tag{19}$$

in analogy to $\theta = \arg\Gamma(i\tau)$ [see Eq. (12)] we have introduced the abbreviation $\chi \overset{\text{def}}{=} \arg\Gamma(i\xi)$.

The regular solution $\psi_{\text{reg}}(r)$ of the Schrödinger equation also depends on the potential at small r values, and vanishes at $r=0$. Bound states exist for energies at which the regular solution matches to the wave function [Eq. (13)] in the region where the potential is already dominated by the two power-law terms of the tail [Eq. (2)], so the condition of quantization, quite generally, is

$$\frac{\psi'_{\text{reg}}}{\psi_{\text{reg}}} = \frac{M'_\kappa}{M_\kappa}. \tag{20}$$

Semiclassical wave functions are defined with the help of the local classical momentum,

$$p(r) = \sqrt{2\mathcal{M}[E - V(r)]}, \tag{21}$$

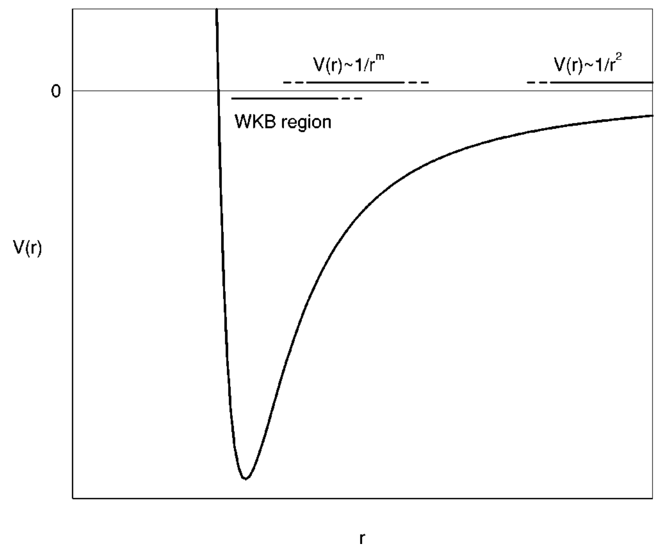

FIG. 1. Schematic illustration of a potential with a tail [Eq. (2)] consisting of an attractive $1/r^2$ term and an attractive $1/r^m$ term. Near-threshold solutions of the Schrödinger equation are well approximated by WKB wave functions in the ''WKB region.'' We assume that this WKB region overlaps with a region of moderate r values where the potential is dominantly described by the $1/r^m$ term.

and WKB wave functions, $\psi_{\text{WKB}} \propto p^{-1/2}\exp[\pm(i/\hbar)\int p\,dr]$, are accurate solutions of the Schrödinger equation when the following condition is fulfilled [2]:

$$\frac{1}{16\pi^2}\left|\left(\frac{d\lambda}{dr}\right)^2 - 2\lambda\frac{d^2\lambda}{dr^2}\right| \ll 1, \tag{22}$$

where $\lambda(r) = 2\pi\hbar/p(r)$ is the (local) de Broglie wavelength. For potentials behaving as $1/r^m$, $m>2$, condition (22) is fulfilled increasingly well as r decreases. We assume that there is a range of r values in the potential well where condition (22) is well fulfilled so that the WKB wave function,

$$\psi_{\text{WKB}}(r) \propto \frac{1}{\sqrt{p(r)}}\cos\left(\frac{1}{\hbar}\int_{r_{\text{in}}}^{r} p(r')\,dr' - \frac{\phi_{\text{in}}}{2}\right) \tag{23}$$

is an accurate solution of the Schrödinger equation, see Fig. 1. The angle ϕ_{in} in Eq. (23) is the reflection phase at the inner classical turning point r_{in}, which is defined so that the WKB wave function (23) agrees with the exact quantum mechanical wave function ψ_{reg} in this ''WKB region''; ϕ_{in} can be taken to be $\pi/2$ if the conditions of the semiclassical limit are fulfilled near the inner classical turning point [30].

The r dependence of both the amplitude and the phase of the wave function (18) is that of the WKB wave function (23) at $E=0$, when the potential near r is given by the shorter-ranged term in the tail alone,

$$\frac{2\mathcal{M}}{\hbar^2}V(r) = -\frac{\beta^{m-2}}{r^m}, \quad p(r) = \hbar\frac{\beta^{(m-2)/2}}{r^{m/2}},$$

$$\frac{1}{\hbar}\int_{r_{\rm in}}^{r} p(r')\,dr' = \text{const} - \rho. \tag{24}$$

If the WKB region overlaps with a range of r values where the potential is dominated by the $1/r^m$ term (see Fig. 1), then the quantization condition can be formulated by matching wave functions (23) and (18) in this range of overlap. We expect the WKB wave function here to be a smooth (analytic) function of energy, so, to order less than κ^2, we can assume $E=0$ in Eq. (23). Equating the cosines in Eqs. (23) and (18) leads to the quantization condition

$$\frac{1}{\hbar}\int_{r_{\rm in}}^{r} p(r')\,dr' - \frac{\phi_{\rm in}}{2} = n\pi - \rho + \frac{\pi}{4} - \delta, \tag{25}$$

where the action integral on the left-hand side is to be taken at threshold, $E=0$. In the region of overlap, where the WKB approximation is accurate *and* the potential is dominated by the $1/r^m$ term, the r dependence of the action integral is compensated for by the term $-\rho$ on the right-hand side of Eq. (25) [cf. Eq. (24)], so the expression

$$I_0 \stackrel{\rm def}{=} \frac{1}{\hbar}\int_{r_{\rm in}}^{r} p(r')\,dr' + \frac{2}{m-2}\left(\frac{\beta}{r}\right)^{(m-2)/2} - \frac{\phi_{\rm in}}{2} - \frac{\pi}{4} \tag{26}$$

is independent of r. With the help of Eq. (19) the quantization condition (25) thus reduces to

$$\tan\left(\theta + \chi + \frac{\pi}{2} - \tau \ln q\right) = \frac{\tan\delta}{\tanh(\xi\pi/2)} = -\frac{\tan I_0}{\tanh(\xi\pi/2)}, \tag{27}$$

which is equivalent to

$$\kappa^2 = \frac{4(m-2)^{4/(m-2)}}{\beta^2}\exp\left\{\frac{2}{\tau}\left[\theta + \chi + \frac{\pi}{2} + \arctan\left(\frac{\tan I_0}{\tanh(\xi\pi/2)}\right)\right]\right\}. \tag{28}$$

The multivalued nature of the arcus tangent in the exponent on the right-hand side of Eq. (28) allows the subtraction of $n\pi$ (n is an integer), and this leads to the known asymptotic ($E\to 0$) behavior of the energies of the dipole series,

$$E_n = -\frac{\hbar^2\kappa_n^2}{2\mathcal{M}} \stackrel{n\to\infty}{=} -F\exp\left(-\frac{2\pi n}{\tau}\right). \tag{29}$$

The theory above now allows us to give an explicit expression for the prefactor F in Eq. (29), namely,

$$F = \frac{2\hbar^2}{\mathcal{M}\beta^2}(m-2)^{4/(m-2)}\exp\left\{\frac{2}{\tau}\left[\theta + \chi + \frac{\pi}{2} + \arctan\left(\frac{\tan I_0}{\tanh(\xi\pi/2)}\right)\right]\right\}. \tag{30}$$

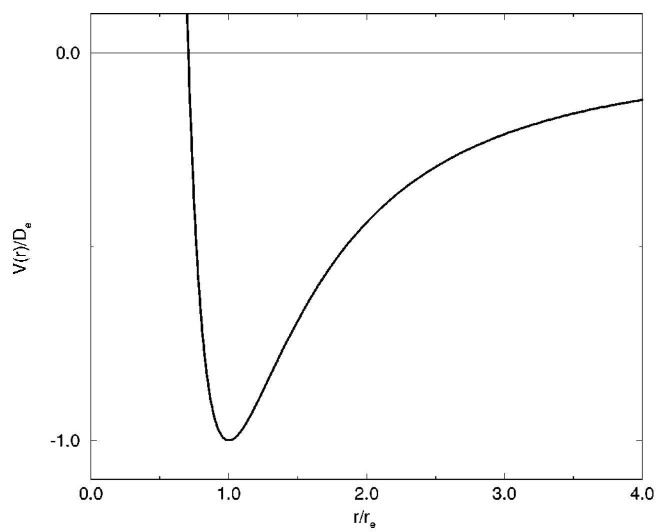

FIG. 2. Potential [Eq. (2)] consisting entirely of a repulsive $1/r^m$ term and an attractive $1/r^2$ term. Here $m=4$ and $g=-\gamma=200$, so the potential corresponds to the case $\eta=5$ studied by Varshni [32]. The potential is given in units of its depth D_e at its minimum r_e; see Eq. (39).

Result (30) holds under the condition that there is a WKB region where condition (22) is well fulfilled, and that this region overlaps with a region of r values where the potential is dominated by the $1/r^m$ term; see Fig. 1. A definite choice of the branch of $\arctan[\tan I_0/\tanh(\xi\pi/2)]$ in Eq. (30) fixes the quantum numbers n assigned to the individual levels. If, in a given potential, we fix the numbering of levels, e.g., by starting with $n=0$ for the ground state, then this determines which branch of the arcus tangent is to be taken. The choice of branch remains undetermined in our present theory based on the near-threshold wave functions.

We now consider the case that the shorter ranged term proportional to $1/r^m$ is repulsive, and that the two terms [Eq. (2)] constitute the whole potential (see Fig. 2). This potential again supports an infinite dipole series if the strength of the (attractive) $1/r^2$ term is large enough ($g>1/4$).

The Schrödinger equation is given by

$$\left[\frac{d^2}{dr^2} + \frac{g}{r^2} - \frac{\beta^{m-2}}{r^m} - \kappa^2\right]\psi(r) = 0. \tag{31}$$

In order to obtain near-threshold wave functions for small and moderate values of r, we neglect the energy term in Eq. (31), and the resulting equation

$$\left[\frac{d^2}{dr^2} + \frac{g}{r^2} - \frac{\beta^{m-2}}{r^m}\right]Z(r) = 0 \tag{32}$$

can be solved with the help of Bessel functions. We keep the abbreviations τ and ξ as defined in Eq. (5) with $\theta = \arg\Gamma(i\tau)$ and $\chi = \arg\Gamma(i\xi)$. The real solution of Eq. (32) which obeys the physical condition of vanishing at the origin is

$$Z(r)=i\exp[-\pi\xi/2]\sqrt{r}H_{i\xi}^{(1)}(i\rho),\quad \rho=\frac{2}{m-2}\left(\frac{\beta}{r}\right)^{(m-2)/2},\tag{33}$$

which behaves as

$$Z(r)\sim\sqrt{\frac{m-2}{\pi}\beta}\left(\frac{r}{\beta}\right)^{m/4}\exp(-\rho)\tag{34}$$

for small r.

For large values of r we use the small argument expansion [29] of the Hankel function $H_{i\xi}^{(1)}$ in Eq. (33), and obtain the leading terms

$$Z(r)\sim\sqrt{\frac{r}{\pi\xi\sinh(\pi\xi)}}\left[(m-2)^{i\xi}e^{i\chi}\left(\frac{r}{\beta}\right)^{i\tau}+(m-2)^{-i\xi}e^{-i\chi}\left(\frac{r}{\beta}\right)^{-i\tau}\right].\tag{35}$$

These leading terms must, except for a common constant of proportionality, agree with the near-threshold limit of wave function (9) as given in Eq. (12), i.e., the ratios of the coefficients of $r^{-i\tau}$ and $r^{i\tau}$ must be the same in Eq. (35) as in Eq. (12). This leads to the condition,

$$\left(\frac{\kappa\beta}{2}\right)^{2i\tau}=(m-2)^{2i\xi}e^{2i(\theta+\chi)},\tag{36}$$

which is equivalent to $\exp[2i(\theta+\chi)]=\exp(2i\tau\ln q)$, with $q=\frac{1}{2}\kappa\beta(m-2)^{-2/(m-2)}$ as in Eq. (19). This corresponds to the quantization condition

$$\kappa_n^2=\frac{4(m-2)^{4/(m-2)}}{\beta^2}\exp\left[\frac{2}{\tau}(\theta+\chi-n\pi)\right],\tag{37}$$

where the multivalued contribution $-n\pi$ on the right-hand side originates from the multivalued nature of the exponentials in Eq. (36). For the energies E_n we again obtain expression (29), but for the prefactor we now have the analytical formula

$$F(m,g)=\frac{2\hbar^2}{\mathcal{M}\beta^2}(m-2)^{4/(m-2)}e^{2(\theta+\chi)/\tau}.\tag{38}$$

The Schrödinger equation (31) was studied by Papp [31] and Varshni [32] for the case $m=4$ with the aim of testing approximation schemes such as the $1/N$ expansion and the WKB approximation. As is customary in molecular physics, the parameters defining the potential are taken as the position r_e of the potential minimum and the depth $D_e=-V(r_e)$ of the well. The energies are normalized to the depth, $\varepsilon_n=E_n/D_e$, and these normalized energies now depend only on the strength g of the attractive $1/r^2$ term, which is related to a parameter called η^2 in Ref. [32]. In terms of our potential parameters g and β, the parameters of Ref. [32] are

$$r_e^2=2\frac{\beta^2}{g},\quad D_e=\frac{\hbar^2g^2}{8\mathcal{M}\beta^2},\quad \eta^2=\frac{g}{8}.\tag{39}$$

For $m=4$ the parameters τ and ξ defined by Eq. (5) are the same, and, according to Eqs. (37) and (38), the threshold behavior of the normalized energies is

$$\varepsilon_n=\frac{E_n}{D_e}=-fe^{-2\pi n/\tau},\quad f=\frac{F(m=4,g)}{D_e}=\frac{e^{4\theta/\tau}}{\eta^4}.\tag{40}$$

For potentials with $\eta=5$, 15, and 25 Varshni [32] listed normalized eigenvalues for quantum numbers from $n=0$ for the ground state to $n=9$, 30, and 55, respectively. In order to demonstrate how these dipole series approach the limiting behavior [Eq. (40)], we plot the logarithms $\ln f_n$ of the effective strength parameters

$$f_n=-\varepsilon_n\times e^{2\pi n/\tau}\tag{41}$$

against the quantum number n. In the limit $n\to\infty$, these effective strengths converge to the strength f in Eq. (40). Here f is defined only to within a factor consisting of an arbitrary integer power of $\exp(2\pi/\tau)$, so $\ln f$ is only defined modulo $2\pi/\tau$. A definite choice of f fixes the quantum numbers n assigned to the individual states [see the discussion after Eq. (30)].

The results are shown in Fig. 3. The values of $\ln f$ following from Eq. (40) for the three values of η are listed in Table I, and shown as dashed horizontal lines in Fig. 3. The convergence of the effective strengths to the respective threshold limits is obvious. This convergence implies that the energies of the near-threshold states are, for growing n, given with increasing (absolute and relative) accuracy by formula (29), with the appropriate prefactor [Eq. (38)], just as the near-threshold energies of a Rydberg series in a Coulomb potential are given with increasing (absolute and relative) accuracy by the Rydberg formula with the appropriate threshold value of the quantum defect [2].

The well known fact that conventional WKB quantization breaks down near threshold, for potentials falling off faster than $1/r^2$ asymptotically, was recently interpreted as a breakdown of Bohr's correspondence principle [33]. The threshold is, however, an unusual place to expect quantum classical correspondence for such potentials [8,10], because it does not correspond to the semiclassical limit. A potential falling off faster than $1/r^2$ supports at most a finite number of bound states, so the limit of infinite quantum numbers, which is fundamental to the usual formulation of Bohr's correspondence principle, cannot be taken. Dipole series form an interesting special case for this discussion. For potentials proportional to $1/r^2$, the accuracy of semiclassical approximations does not depend on energy—the semiclassical limit is reached for large absolute values of the strength parameter [2]. However, a sufficiently attractive $1/r^2$ potential tail with a fixed strength parameter $g>1/4$ does support an infinite number of bound states. As is obvious from the tables in Ref. [32], the relative errors of the energy eigenvalues obtained via conventional WKB quantization become

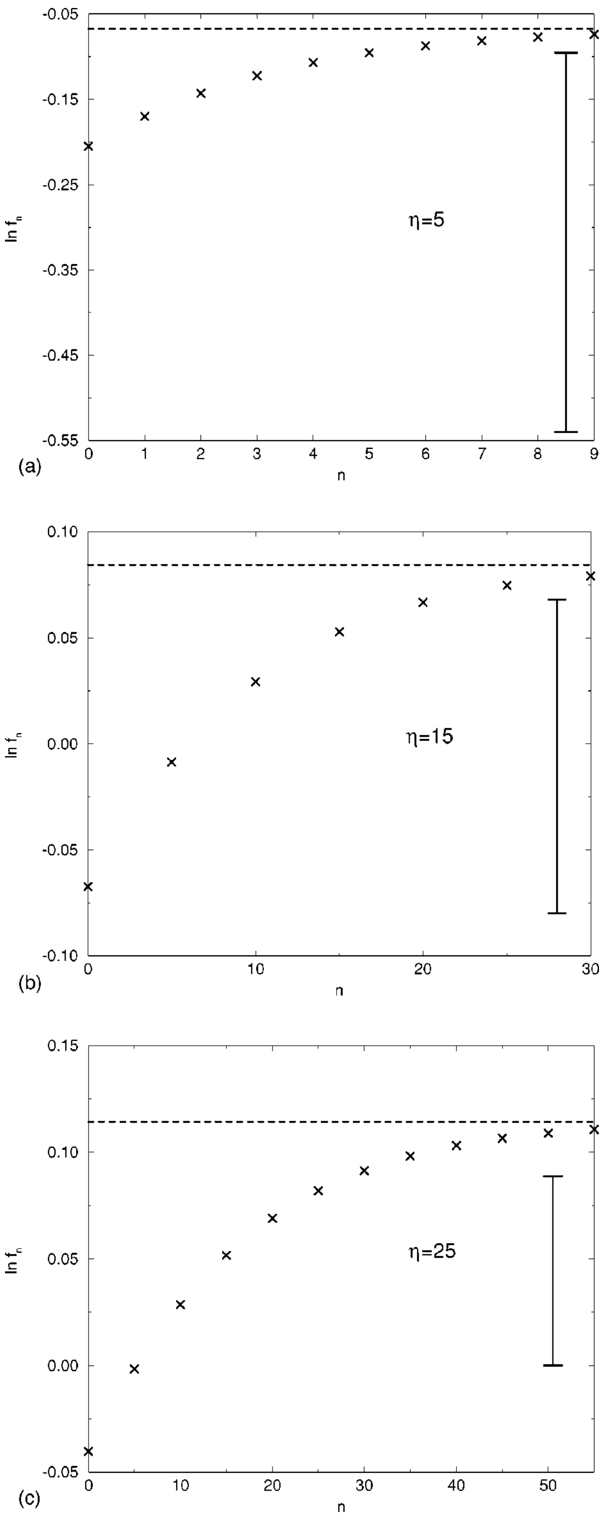

FIG. 3. Logarithmic plot of the effective strength parameters f_n [Eq. (41)] for the (normalized) energy eigenvalues ε_n calculated by Varshni [32] for a potential [Eq. (2)] consisting entirely of a repulsive $1/r^4$ term and an attractive $1/r^2$ term for $\eta = 5$, 15, and 25. The dashed horizontal line in each panel shows the threshold limit $\ln f$ of the $\ln f_n$ as the behavior of the energies approaches the dipole series form [Eq. (40)]; also see Table I. This limit is defined only modulo $2\pi/\tau$, and the magnitudes of $2\pi/\tau$ for the various values of η are shown as vertical bars in the respective panels.

TABLE I. Values of $\ln f$ for the threshold limits f which determine, via Eq. (40), the explicit values of the normalized energies in the dipole series generated by the Schrödinger equation (31) for $m=4$.

η	g	$2\pi/\tau$	$\ln f$
5	200	0.444566	-0.0675707
15	1800	0.148106	$+0.0843669$
25	5000	0.0888599	$+0.1142865$

larger with increasing quantum numbers for all potentials studied. [Note, however, that higher-order WKB results are very accurate for all quantum numbers.] Thus dipole series in potentials with an attractive $1/r^2$ tail are a genuine example where the naive expectation that semiclassical approximations necessarily improve in the limit $n \to \infty$ is not fulfilled. This naive interpretation of Bohr's correspondence principle fails in the present case. Here, as elsewhere, the correspondence principle refers to the semiclassical limit. For the attractive $1/r^2$ potential tail, the semiclassical limit can be realized by taking the limit of large strength parameters, independent of energy. For a discussion of potential tails falling off faster than $1/r^2$; see Refs. [8,10].

III. TUNNELING

When the $1/r^2$ term is repulsive and the shorter-ranged $1/r^m$ term is attractive, then potential (2) represents a barrier typical for the radial Schrödinger equation with nonvanishing angular momentum; see Fig. 4. The Schrödinger equation for this barrier is

$$\left[\frac{d^2}{dr^2} - \frac{\gamma}{r^2} + \frac{\beta^{m-2}}{r^m} + k^2\right]\psi(r) = 0, \quad \gamma > 0. \tag{42}$$

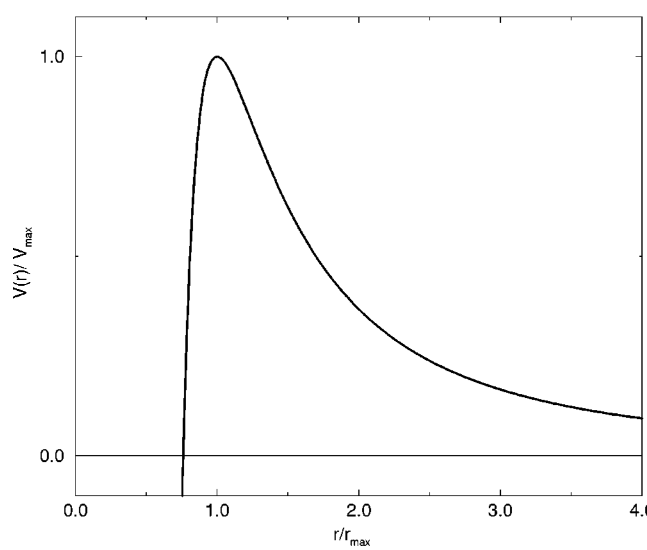

FIG. 4. Potential barrier consisting of a repulsive $1/r^2$ term and an attractive $1/r^m$ term. Here $m=6$ as for a van der Waals interaction, and the strength of the $1/r^2$ term corresponds to a centrifugal potential with angular momentum quantum number $l=1$.

For an angular momentum quantum number l, the strength of the $1/r^2$ term is $\gamma=l(l+1)$.

In the following we shall calculate the threshold behavior of the probability for transmission from a region of low-r values to the left of the barrier to large-r values beyond the barrier. Reflection by and transmission through the potential tail [Eq. (2)] can also be discussed in the absence of the centrifugal term, $\gamma=0$ [9,34], as long as there is a range of small r values where Eq. (22) is well fulfilled so that incoming and reflected WKB waves are accurate solutions of the Schrödinger equation. The following theory can be applied for $\gamma=0$, and even for a *weakly attractive* $1/r^2$ term, meaning that γ can be negative but must be larger than $-1/4$.

At threshold, $E=0$, the Schrödinger equation (42) is

$$\left[\frac{d^2}{dr^2}-\frac{\gamma}{r^2}+\frac{\beta^{m-2}}{r^m}\right]W(r)=0. \tag{43}$$

In analogy to Eq. (5), we introduce the abbreviations

$$\mu\stackrel{\text{def}}{=}\sqrt{\gamma+\frac{1}{4}},\quad \nu\stackrel{\text{def}}{=}\frac{2\mu}{m-2}=\frac{2}{m-2}\sqrt{\gamma+\frac{1}{4}}. \tag{44}$$

The condition $\gamma>-1/4$ mentioned above implies that both μ and ν are positive real numbers. Two linearly independent solutions of Eq. (43) are

$$W_{1;2}(r)=\sqrt{r}J_{\pm\nu}(\rho),\quad \rho=\frac{2}{m-2}\left(\frac{\beta}{r}\right)^{(m-2)/2}. \tag{45}$$

The asymptotic ($r\to\infty$) behavior of solutions (45) is

$$W_{1;2}(r)\sim\frac{(m-2)^{\mp\nu}}{\Gamma(1\pm\nu)}\sqrt{r}\left(\frac{r}{\beta}\right)^{\mp\mu}\left(1-\frac{(\beta/r)^{m-2}}{(m-2)^2(1\pm\nu)}\right). \tag{46}$$

For large values of r the $1/r^2$ term dominates the potential, and the Schrödinger equation (42) corresponds to

$$\left[\frac{d^2}{dr^2}-\frac{\gamma}{r^2}+k^2\right]U=0. \tag{47}$$

The solutions of Eq. (47) are functions of kr only, and the solution which describes an outward traveling wave is

$$U(kr)=\exp\left(i\frac{\pi}{2}\mu\right)\sqrt{kr}H_\mu^{(1)}(kr), \tag{48}$$

which behaves asymptotically ($kr\to\infty$) as

$$U(kr)\sim\sqrt{\frac{2}{\pi}}\exp\left[i\left(kr-\frac{\pi}{4}\right)\right]. \tag{49}$$

Near threshold, $kr\to 0$, the leading contribution to Eq. (48) is [29]

$$U(kr)\stackrel{kr\to 0}{\sim}-i\frac{\sqrt{2}}{\pi}e^{i\pi\mu/2}\Gamma(\mu)\left(\frac{kr}{2}\right)^{(1/2)-\mu}. \tag{50}$$

The r dependence of Eq. (50) agrees with the r dependence of the leading asymptotic ($r\to\infty$) behavior of the solution $W_1(r)$ [see Eq. (46)], so in the near-threshold limit $k\to 0$ these solutions can be matched according to

$$U(kr)\stackrel{kr\to 0}{=}LW_1(r), \tag{51}$$

and the k-dependent coefficient is given by

$$L=\sqrt{k}\,\frac{e^{i\pi\mu/2}}{i\pi}\Gamma(1+\nu)\Gamma(\mu)(m-2)^\nu\left(\frac{k\beta}{2}\right)^{-\mu}. \tag{52}$$

To the left of the barrier, $r\to 0$, the large argument expansion of the Bessel function $J_\nu(\rho)$ yields

$$W_1(r)\sim\sqrt{\frac{m-2}{\pi}\beta}\left(\frac{r}{\beta}\right)^{m/4}\cos\left(\rho-\frac{\pi}{2}\nu-\frac{\pi}{4}\right), \tag{53}$$

so the wave function $LW_1(r)$ has the form[1]

$$LW_1(r)\stackrel{r\to 0}{\sim}\sqrt{\frac{m-2}{4\pi}\beta}\left(\frac{r}{\beta}\right)^{m/4}L\cdot\left(e^{-i\pi\nu/2}e^{i(\rho-\pi/4)}+e^{+i\pi\nu/2}e^{-i(\rho-\pi/4)}\right). \tag{54}$$

The amplitude and phase of the two terms in Eq. (54) correspond to the amplitude and phase of leftward traveling (reflected) and rightward traveling (incoming) waves in the WKB approximation, which becomes increasingly accurate for small-r values where the $1/r^m$ term dominates the potential. The associated current densities, $J=\mathrm{Im}[(\hbar/\mathcal{M})\psi^* d\psi/dr]$, are

$$J_{\text{in/refl}}=\frac{\hbar}{4\pi\mathcal{M}}(m-2)|L|^2, \tag{55}$$

[1]In a recent paper, Gao [35] studied potential tails consisting of a centrifugal term and an attractive term proportional to $1/r^m$, $m=6$, and he found the following rule: If the potential well supports a zero-energy bound state for an angular momentum quantum number l_b, it will also do so for $l=l_b\pm 4$, $l_b\pm 8,\dots$ (as long as $l\geqslant 0$). This rule and its generalization to any $m>2$ follow immediately from the properties of the wave function W_1 [Eq. (45)], which solves the Schrödinger equation (43) with the correct asymptotic (large r) boundary conditions and is to be matched to the regular solution coming from the origin. To the left of the barrier, $W_1(r)$ becomes proportional to Eq. (53), and depends on l only via the contribution $-\nu\pi/2=-(l+\frac{1}{2})\pi/(m-2)$ to the argument of the cosine, so the wave function is invariant up to a sign when l changes by an integral multiple of $m-2$. If matching to the regular solution yields a bound state at threshold for one angular momentum quantum number l_b, then it will do so also for $l=l_b\pm(m-2)$, $l_b\pm 2(m-2),\dots$ ($l\geqslant 0$). An important condition for this rule to hold is, of course, that the wave function to the left of the matching point be essentially unaffected by the centrifugal potential; for a potential well of finite depth this cannot be fulfilled for an arbitrarily large l.

TABLE II. Values of the coefficient [Eq. (58)] of $(k\beta)^{2\mu}$ in the leading term describing the near-threshold behavior of the transmission probabilities [Eqs. (57)] through a potential barrier consisting of an attractive $1/r^m$ potential $(m>2)$ and a repulsive $1/r^2$ (centrifugal) potential with a strength parameter γ corresponding to angular momentum quantum number l, $\mu=\sqrt{\gamma+1/4}=l+1/2$.

$P(m,\gamma)$	$m=3$	$m=4$	$m=5$	$m=6$
$l=0$	4π	4	2.52537	1.91196
$l=1$	$\pi/9$	4/9	0.465421	0.464911
$l=2$	$\pi/32400$	4/2025	0.00527976	0.00849758
$l=3$	0.219870×10^{-8}	0.161250×10^{-5}	0.0000143161	0.0000421688
$l=4$	0.865576×10^{-14}	0.406273×10^{-9}	0.144770×10^{-7}	0.856395×10^{-7}
$l=5$	0.883151×10^{-20}	0.414522×10^{-13}	0.687112×10^{-11}	0.878061×10^{-10}
$l=6$	0.299916×10^{-26}	0.202710×10^{-17}	0.176390×10^{-14}	0.517031×10^{-13}
$l=7$	0.402416×10^{-33}	0.533097×10^{-22}	0.269760×10^{-18}	0.190840×10^{-16}
$l=8$	0.241743×10^{-40}	0.819834×10^{-27}	0.263645×10^{-22}	0.470489×10^{-20}
$l=9$	0.715162×10^{-48}	0.785816×10^{-32}	0.173684×10^{-26}	0.812985×10^{-24}
$l=10$	0.112305×10^{-55}	0.493600×10^{-37}	0.804279×10^{-31}	0.102260×10^{-27}

and they are equal to leading order, because the transmitted current density is of higher order in k. The transmitted wave traveling rightward at large r values is given by Eq. (49), and the associated current density is

$$J_{\text{trans}}=\frac{2\hbar k}{\pi\mathcal{M}}. \tag{56}$$

In order to obtain the current density of the reflected wave to an accuracy sufficient to fulfill the continuity condition, $J_{\text{in}}=J_{\text{refl}}+J_{\text{trans}}$, we would have to include higher-order terms in the solution of the Schrödinger equation, in particular the contribution proportional to $(kr)^{1/2+\mu}$ in the near-threshold limit [36]. From Eqs. (56) and (55) the transmission probability $T=J_{\text{trans}}/J_{\text{in}}$ is, to leading order,

$$T=\frac{4\pi^2}{(m-2)^{2\nu}\mu\nu[\Gamma(\nu)\Gamma(\mu)]^2}\left(\frac{k\beta}{2}\right)^{2\mu}\overset{\text{def}}{=}P(m,\gamma)(k\beta)^{2\mu}. \tag{57}$$

The parameters μ and ν are defined in Eq. (44), and μ is related to the angular momentum quantum number l of the centrifugal potential by $\mu=\sqrt{\gamma+1/4}=l+1/2$. The proportionality of T to $k^{2\mu}$, i.e., to $E^{l+1/2}$, is simply an expression of Wigner's threshold law [2]. Since β is the only length scale in the Schrödinger equation, the dimensionless transmission probability is (to leading order) naturally proportional to $(k\beta)^{2\mu}$. The derivation above, however, also gives, for all potential barriers consisting of a repulsive (or weakly attractive) $1/r^2$ term and an attractive $1/r^m$ term $(m>2)$, the exact analytical expression for the coefficient of $(k\beta)^{2\mu}$:

$$P(m,\gamma)=\frac{4\pi^2}{(m-2)^{2\nu}2^{2\mu}\mu\nu[\Gamma(\nu)\Gamma(\mu)]^2}. \tag{58}$$

The numerical values of P are listed in Table II for $m=3$, 4, 5, and 6, and for strength parameters γ corresponding to angular momentum quantum numbers $l=0,\ldots,10$.

When the strength of the $1/r^2$ term vanishes, $\gamma=0$, we have $\mu=1/2$ and $\nu=1/(m-2)$; result (57) for this case agrees with the result derived for the reflection probability $1-T$ of an attractive $1/r^m$ potential tail [9,34]. For arbitrary γ $(>-1/4)$ and the special case $m=4$, the Schrödinger equation (42) can be solved analytically with the help of Mathieu functions [20]. The transmission probability near $E=0$ can be derived from the asymptotic ($r\to0$ and $r\to\infty$) forms of the wave functions given in Ref. [20], and this leads exactly to result (57) with $m=4$. Note, however, that the aim of Ref. [20] was to derive scattering lengths and effective range parameters based on an expansion of the cotangent of the scattering phase shifts as functions of the asymptotic wave number k. This expansion is not really valid for potentials behaving like Eq. (2), and the number of usable leading terms it contains depends on the angular momentum quantum number l and on the power m of the attractive $1/r^m$ term. In contrast, formula (57) derived above is not restricted in such a way. It is valid for any strength parameter $\gamma>-1/4$ and for any, not necessarily integer, power $m>2$.

The derivation above requires the compatibility of approximations (43) and (47) to the Schrödinger equation (42) for a common range of r values. In analogy to Eq. (17) this leads to the condition

$$k\beta\ll|\gamma|^{(1/2)+[1/(m-2)]}, \tag{59}$$

which is fulfilled in the limit $k\to0$ for any finite value of $|\gamma|$. As mentioned above, result (57) also gives the correct leading behavior for the case $\gamma=0$ [9,34].

Tunneling probabilities are frequently approximated with the help of the WKB formula [37],

$$T_{\text{WKB}}=\exp(-2I),\quad I=\int_{r_{\text{in}}}^{r_{\text{out}}}\frac{1}{\hbar}|p(r)|dr, \tag{60}$$

where r_{in} and r_{out} are the two classical turning points, between which the local classical momentum $p(r)$ is purely imaginary. For potentials falling off faster than $1/r^2$, formula (60) fails near threshold, because it yields a finite value at

$E=0$, whereas the exact tunneling probability vanishes in this limit, as pointed out in Ref. [38]. For a potential barrier asymptotically equal to γ/r^2 [times $\hbar^2/(2\mathcal{M})$], the WKB tunneling probability [Eq. (60)] is proportional to $k^{2\sqrt{\gamma}}$ near threshold, so the correct energy dependence $T\propto E^{\mu}$ can be recovered with the help of the Langer modification $\gamma\rightarrow\gamma+1/4$, which amounts to replacing $l(l+1)$ by $(l+1/2)^2$ for the centrifugal potential [2,37]. Criticisms and improvements of the Langer modification were recently discussed in various contexts [2,19,30,39]. The present derivation of the asymptotically ($E\rightarrow 0$) exact formula for the transmission probability for potential barriers of the special form [Eq. (2)] allows us to give a founded judgement on the accuracy of the usual procedure involving the WKB formula [Eq. (60)] with the Langer modified potential.

The integrand of the action integral in Eq. (60) is

$$\frac{1}{\hbar}|p(r)|=\sqrt{\frac{\mu^2}{r^2}-\frac{\beta^{m-2}}{r^m}-k^2}, \tag{61}$$

where we have invoked the Langer modification and replaced γ by $\gamma+1/4=\mu^2$. Note that the condition $\gamma>-1/4$, for which the above theory is applicable, corresponds to the condition that the *Langer modified* potential is asymptotically repulsive. We obtain an upper bound for the integral I if we neglect one of the subtracted terms in the square root. For a given point $\tilde{r}$ with $r_{\rm in}<\tilde{r}<r_{\rm out}$, we thus have

$$I\leqslant\int_{r_{\rm in}}^{\tilde{r}}\sqrt{\frac{\mu^2}{r^2}-\frac{\beta^{m-2}}{r^m}}dr+\int_{\tilde{r}}^{r_{\rm out}}\sqrt{\frac{\mu^2}{r^2}-k^2}dr. \tag{62}$$

Inequality (62) remains valid if we replace the inner classical turning point $r_{\rm in}$ by its threshold value $r_{\rm in0}$ and the outer classical turning point $r_{\rm out}$ by the value $r_{\rm out0}$ obtained by neglecting the $1/r^m$ term in the potential:

$$r_{\rm in0}=\frac{\beta}{\mu^{2/(m-2)}}\leqslant r_{\rm in},\quad r_{\rm out0}=\frac{\mu}{k}\geqslant r_{\rm out}. \tag{63}$$

The right-hand side of inequality (62) can then be easily evaluated analytically. We choose the value of $\tilde{r}$ such, that the two terms neglected in the respective integrals in Eq. (62) have equal magnitudes at $\tilde{r}$:

$$\frac{\beta^{m-2}}{\tilde{r}^m}=k^2,\quad k\tilde{r}=(k\beta)^{1-2/m}=(k\beta)^{1-2/m}. \tag{64}$$

The leading orders of the approximated action integral are then

$$I_{\rm approx}\overset{\rm def}{=}\int_{r_{\rm in0}}^{\tilde{r}}\sqrt{\frac{\mu^2}{r^2}-\frac{\beta^{m-2}}{r^m}}dr+\int_{\tilde{r}}^{r_{\rm out0}}\sqrt{\frac{\mu^2}{r^2}-k^2}dr$$
$$=\frac{m\mu}{m-2}\left[\ln\left(\frac{2\mu}{(k\beta)^{1-2/m}}\right)-1+O((k\beta)^{2-4/m})\right]. \tag{65}$$

Since $I_{\rm approx}$ is an upper bound for the action integral entering the WKB expression [Eq. (60)], the corresponding expression $\exp(-2I_{\rm approx})$ is a lower bound for the WKB approximation to the tunneling probability:

$$T_{\rm WKB}\geqslant\exp(-2I_{\rm approx})$$
$$=\left(\frac{e}{2\mu}\right)^{2m\mu/(m-2)}(k\beta)^{2\mu}[1+O((k\beta)^{2-4/m})]. \tag{66}$$

The coefficient of $(k\beta)^{2\mu}$ on the right-hand side of Eq. (66) is larger than the coefficient P of $(k\beta)^{2\mu}$ in the exact expression [Eq. (57)] for the near-threshold tunneling probability. The usual WKB treatment overestimates the exact tunneling probability by at least the factor

$$G\overset{\rm def}{=}\lim_{k\rightarrow 0}\frac{\exp(-2I_{\rm approx})}{T}=\left(\frac{e^{\mu+\nu}\Gamma(\mu)\Gamma(\nu)}{2\pi\mu^{\mu-1/2}\nu^{\nu-1/2}}\right)^2. \tag{67}$$

For large values of the strength γ of the $1/r^2$ term in the potential, μ and ν are also large and we can express the gamma functions in Eq. (67) via Stirling's formula [29]. This yields

$$G\overset{\gamma\rightarrow\infty}{\sim}1+\frac{m}{12\mu}+O\left(\frac{1}{\mu^2}\right), \tag{68}$$

showing that the WKB treatment [with the additional approximation according to Eq. (65)] becomes exact for large angular momentum quantum numbers.

For smaller strength parameters γ corresponding to lower angular momentum quantum numbers, the error in the conventional WKB treatment of the tunneling probability can, however, be quite large. For $m=3$, 4, 5, and 6, the numerical values of G are displayed in Fig. 5 as functions of μ ($\equiv l+1/2$). For a given strength of the $1/r^2$ term in the potential, the relative error in the WKB tunneling probability increases with the power m of the shorter-ranged $1/r^m$ term, and it becomes proportional to m for large m values. For the realistic and important case $m=6$ and $\mu=3/2$, corresponding to a van der Waals interaction with an $l=1$ centrifugal potential, the WKB tunneling probability is too large by at least 38%.

Because of the large errors in the WKB tunneling probabilities for low partial waves, such methods should be regarded critically in the near-threshold regime. Consider, e.g., a reaction leading to a compound particle, where the formation cross section is typically given by an expression of the form [40,41]

$$\sigma_C=\sum_{l=0}^{\infty}\sigma_l=\sum_{l=0}^{\infty}\frac{(2l+1)\pi}{k^2}T_l. \tag{69}$$

Here T_l is essentially the probability of transmission through the effective potential barrier in partial wave l. We mention in passing that the transmission probability through a potential barrier does not depend on the direction of propagation [42]. Due to Wigner's threshold law, the contributions from low partial waves dominate the cross section (69) near threshold, so the large errors from these partial waves will

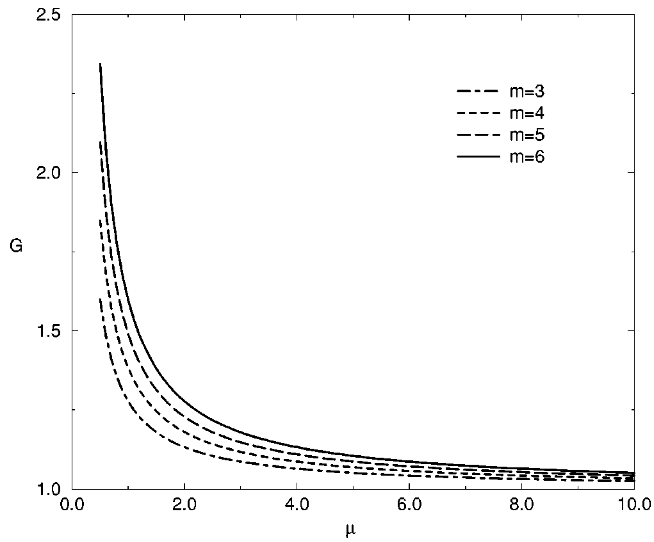

FIG. 5. Behaviour of G [Eq. (67)] as function of the parameter μ for $m=3$, 4, 5, and 6. For a potential barrier consisting of an attractive $1/r^m$ potential and centrifugal potential with an angular momentum quantum number $l=\mu-1/2$, G is a lower bound for the factor by which the conventional calculation of transmission probabilities via the WKB formula [Eq. (60)] and the Langer modification of the potential overestimates the exact near-threshold transmission probabilities [Eq. (57)].

affect the whole sum. Accurate calculations for the simplest case of a sharp edged centrifugal barrier were already presented in Ref. [41]. Our present theory offers the exact result for the near-threshold transmission probability in the more realistic case of an additional $1/r^m$ potential, which can describe the interaction due to polarization in a two-body atomic system.

Another example for the importance of transmission probabilities is the decay of a metastable system trapped by a potential barrier. The standard semiclassical expression for the width Γ of such a resonant state is [43]

$$\Gamma=\frac{\hbar}{t_{\mathrm{cl}}}T, \tag{70}$$

where T is the transmission probability through the barrier, and t_{cl} is the classical period of oscillation of the particle in the classically allowed region to the left of the barrier. It has been frequently observed and again pointed out recently [44] that this approximation is not accurate enough when the WKB approximation [Eq. (60)] is used for T. If the semiclassical approximation is applicable in the classically allowed region to the left of the barrier, then formula (70) should, however, yield increasingly accurate results toward threshold, provided the exact expression [Eq. (57)] is used for the transmission probability (assuming the potential barrier is of the appropriate type). This is particularly useful for extremely narrow near-threshold resonances for which the direct numerical solution of the Schrödinger equation presents a problem.

IV. CONCLUSION

We have presented a comprehensive study of near-threshold properties for an attractive or repulsive $1/r^2$ potential in conjunction with a shorter-ranged $1/r^m$ contribution to the potential tail, $m>2$. For an attractive $1/r^2$ potential supporting an infinite dipole series of bound states, we have derived an explicit expression for the threshold value of the pre-exponential factor determining the absolute positions of the energy levels according to Eq. (29). For a potential tail with an attractive $1/r^m$ term, the WKB approximation becomes increasingly accurate for small distances r, and the prefactor [Eq. (30)] depends on the threshold value of an appropriate WKB integral; see Eq. (26). For a potential consisting entirely of an attractive $1/r^2$ term and a repulsive $1/r^m$ term ($m>2$), we have given the exact analytical expression [Eq. (38)] for the pre-exponential factor, and we demonstrated the convergence of numerically calculated energy levels [32] to the appropriate dipole series behavior; see Fig. 3.

A repulsive $1/r^2$ potential in conjunction with an attractive $1/r^m$ term ($m>2$) is a realistic representation of a potential barrier formed by a centrifugal potential and a shorter-ranged polarization potential. For this case we have derived the exact analytical expression [Eq. (57)] for the near-threshold behavior of the probability for transmission through the barrier. It contains the $k^{2\mu}\propto E^{l+1/2}$ behavior of Wigner's threshold law, as well as the analytical expression for the coefficient of this leading term; see Eq. (58). The conventional treatment, based on the WKB formula for the transmission probability and the Langer modification of the potential, gives the right energy dependence, but a coefficient which is too large. We have derived a lower bound [Eq. (67)] for the factor by which the conventional WKB treatment overestimates the exact tunneling probability near threshold. This factor approaches unity for large strengths of the $1/r^2$ term (large angular momentum quantum numbers l), but for fixed l it becomes arbitrarily large with increasing powers m of the $1/r^m$ term. For the realistic example corresponding to $l=1$ and a van der Waals potential ($m=6$), the WKB result overestimates the exact tunneling probability by at least 38%.

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